Surface acoustic waves in the continuous spectrum of Bloch waves in piezoelectric one-dimensional phononic crystals

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This paper theoretically investigates surface acoustic waves (SAWs) which emerge within the continuous spectrum of bulk Bloch waves in piezoelectric one-dimensional phononic crystals. Accordingly, these SAWs may be treated as an example of the bound states in the continuum (BIC). The equations which determine the existence of such BIC-SAWs have been derived. Unlike SAWs in the frequency intervals forbidden for bulk Bloch waves, BIC-SAWs are governed not by a single purely real dispersion equation but by sets of equations, so BIC-SAWs prove to be robust only to a consistent change of a definite number of free parameters characterizing the wave propagation. The form of the derived equations allows the establishment of the conditions on the frequency and other parameters under which the BIC-SAW exists. The number of conditions depends on the number of bulk waves in the frequency interval under consideration. In the case of generic crystallographic symmetry, there are three, five, and seven conditions which have to be fulfilled for a BIC-SAWs to coexist with one pair, two pairs, and three pairs of bulk Bloch waves, respectively. It is shown that the crystallographic symmetry may reduce the number of conditions to two, three and four, respectively. Numerical computations confirm analytic results.

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I. INTRODUCTION

During last time in various areas of physics there has been a permanent interest in the investigation of a special type of eigenmodes called bound states in the continuum (BIC). These states emerge in different systems both discrete, such as isolated atoms or resonator structures, and continuous, e.g., in usual solids. Specific features of BICs is that they are localized within a domain and have frequencies falling into the continuous spectrum of waves freely propagating in the surrounding space [1–12].

Surface acoustic waves (SAWs) are an example of one-dimensional bound states in solids in the sense that they are localized near the boundary along the normal to it, so that their amplitudes vanish in the depth of substrates [13]. Usually SAWs exist outside the frequency intervals of bulk waves. For instance, these are the Rayleigh wave in isotropic homogeneous substrates and the Love wave in an isotropic layer deposited on an isotropic substrate. However, SAWs may emerge within the spectrum of bulk waves as well. Such BIC-SAWs are also called supersonic SAWs with the fact in mind that their velocity proves to be larger than the velocity along the boundary of bulk waves of certain branches. Accordingly, SAWs in the range of bulk wave nonexistence are called subsonic since their velocity is less than the bulk wave velocities.

It has been discovered, mainly by numerical computations aimed at searching for leaky SAWs with minimal attenuation, that BIC-SAWs exist in various structures [13–24]. BIC-SAWs may arise owing to crystallographic symmetry, e.g., when the sagittal plane coincides with the plane of symmetry since then either the BIC-SAW are in-plane polarized whereas bulk waves are purely shear polarized or vice versa. However, a more curious option is when the BIC-SAW and bulk waves possess all the three components of mechanical displacement and traction.

In Refs. [25–29], an analytical method has been developed to analyze subsonic SAWs in a variety of structures of generic crystallographic symmetry without necessity of solving explicitly even the wave equation. It has allowed the establishment of the maximum number and, in certain cases, the existence conditions of subsonic SAWs on nonpiezoelectric, piezoelectric, and multiferroic half-infinite homogeneous substrates [25,26,30–32] and on the contact of two half-infinite media [24,33–36]. In Refs. [37–41], this method has been generalized to SAWs in forbidden zones of one-dimensional (1D) phononic crystals. These SAWs are counterparts of subsonic SAWs in homogeneous media in that they emerge in frequency intervals forbidden for the existence of delocalized freely propagating Bloch waves.

The BIC-SAW problem proves to be more involved because the number of localized modes at frequencies allowed for bulk waves is less than the number of boundary conditions. However it has been possible to establish certain general properties of BIC-SAWs, such as the conditions constraining the existence of BIC-SAWs on half-infinite homogeneous substrate [42,43] and on nonpiezoelectric 1D phononic crystals [44]. In Refs. [20,21,23,45], the number of equations governing BIC-SAWs for certain symmetric orientations of nonpiezoelectric and piezoelectric substrates coated with layers as well as for generic orientations of nonpiezoelectric substrates coated with layers has been established. It should be mentioned that in phononic crystals BIC-SAWs can exist when all the materials are elastically isotropic, in

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contrast to the case of homogeneous isotropic half-infinite substrates.

The present paper analyzes the existence conditions for BIC-SAWs in piezoelectric 1D phononic crystals. It is worth noting that even in the case of weak piezoeffect this problem cannot be approached via a perturbation theory applied to the equations derived earlier in [44] for BIC-SAWs in nonpiezoelectric phononic crystals. Due to piezoelectric coupling an additional mode, the mode of electric potential, is involved in BIC-SAWs and additional boundary conditions have to be fulfilled, so it is impossible to decide without a special analysis whether these changes entail additional constraints on the existence of BIC-SAWs.

Our paper is organized as follows. In Sec. II, certain properties of plane waves are discussed. In Sec. III, the boundary conditions are formulated. Sections IV and V derives equations on BIC-SAWs and analyze the number of conditions on the existence of these waves in phononic crystals. In Sec. VI, it is shown that the crystallographic symmetry may reduce the number of conditions for BIC-SAWs. In Sec. VII, numerical computations of BIC-SAWs branches are discussed. These computations validate the conclusions obtained analytically in previous sections. Section VIII summarizes the results. The appendices give relations used in Secs. IV–VI.

II. PLANE WAVES IN LAYERED MEDIA

Let a piezoelectric medium occupy the half-space $z \equiv \mathbf{nr} > 0$, where $\mathbf{r}$ is the radius vector and $\mathbf{n}$ is a unit vector. We assume that this medium is inhomogeneous only along the direction of $\mathbf{n}$ and consider electroacoustic waves

$$\begin{pmatrix} \mathbf{u}(\mathbf{r},t) \\ \varphi(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} \boldsymbol{A}(z) \\ \Phi(z) \end{pmatrix} e^{i[k(\mathbf{mr})-\omega t]}, \tag{1}$$

which propagate along the direction of the unit vector $\mathbf{m}$ ($\mathbf{m}\perp\mathbf{n}$) with the frequency ω and wave number k. The functions $\boldsymbol{A}(z)$ and $\Phi(z)$ describe, respectively, the dependence of the mechanical displacement $\mathbf{u}(\mathbf{r},t)$ and electric potential $\varphi(\mathbf{r},t)$ on $z = \mathbf{nr}$.

The traction $\boldsymbol{F}(z) = \hat{\boldsymbol{\sigma}}\mathbf{n}$, where $\hat{\boldsymbol{\sigma}}(z)$ is the tensor of stresses produced by wave (1), and the projection $\mathbb{D}(z) = \mathbf{n}\boldsymbol{D}$ of the electric displacement $\boldsymbol{D}(z)$ may be found in parallel with $\boldsymbol{A}(z)$ and $\Phi(z)$ by solving the system of eight equations [26,31,38]

$$\frac{1}{i}\frac{d\boldsymbol{\xi}}{dz} = \hat{\mathbf{N}}\boldsymbol{\xi}, \tag{2}$$

where $\hat{\mathbf{N}}$ is an 8×8 matrices (see Appendix A) and $\boldsymbol{\xi}$ is an eight component vector column

$$\boldsymbol{\xi}(z) = \begin{pmatrix} \boldsymbol{U} \\ \boldsymbol{V} \end{pmatrix}, \quad \boldsymbol{U}(z) = \begin{pmatrix} \boldsymbol{A} \\ \Phi \end{pmatrix}, \quad \boldsymbol{V}(z) = \begin{pmatrix} \boldsymbol{L} \\ D \end{pmatrix}, \tag{3}$$

where $D = i\mathbb{D}$ and $\boldsymbol{L} = i\boldsymbol{F}$.

In layered structures $\hat{\mathbf{N}}(z) = \hat{\mathbf{N}}_j$ for $z_{j-1} < z < z_j$, where $\hat{\mathbf{N}}_j$ is the $\hat{\mathbf{N}}$ matrix of the jth layer occupying the space $z_{j-1} < z < z_j$. The vector $\boldsymbol{\xi}(z)$ is a continuous function of z because it is assumed that the rigid contact is realized at all the interlayer boundaries. Therefore a solution to (2) for $z > 0$ lying inside the jth layer can be written in the form

$$\boldsymbol{\xi}(z) = \hat{\mathbf{M}}_z(z)\boldsymbol{\xi}_0, \tag{4}$$

where $\boldsymbol{\xi}_0 = \boldsymbol{\xi}(0)$ and $\hat{\mathbf{M}}_z(z)$ is a transfer matrix,

$$\hat{\mathbf{M}}_z(z) = e^{i(z-z_{j-1})\hat{\mathbf{N}}_j} \prod_{s=1}^{j-1} e^{ih_s\hat{\mathbf{N}}_s}, \tag{5}$$

where h_s is the thickness of the sth layer. In 1D phononic crystals partial solutions to (2) are classified by linking them to eigenvectors of the transfer matrix $\hat{\mathbf{M}}$ of unit cell,

$$\hat{\mathbf{M}} = \hat{\mathbf{M}}_z(l) = \prod_{j=1}^{n} e^{ih_j\hat{\mathbf{N}}_j}, \tag{6}$$

where n is the number of layers per period and $l = \sum_{j=1}^{n} h_j$ is the length of period. This link is established by letting $\boldsymbol{\xi}_0 = \boldsymbol{\zeta}_\alpha$, where $\boldsymbol{\zeta}_\alpha$ is the eigenvector of $\hat{\mathbf{M}}$ corresponding to an eigenvalue γ_α. In this case, the vector $\boldsymbol{\xi}_\alpha(z) = \hat{\mathbf{M}}_z(z)\boldsymbol{\zeta}_\alpha$ at the edge $z_n = nl$ of the nth period takes the value $\boldsymbol{\xi}_\alpha(z_n) = \gamma_\alpha^n\boldsymbol{\zeta}_\alpha$.

If $|\gamma_\alpha| \neq 1$, then the amplitude of the mode α decreases ($|\gamma_\alpha| < 1$) or increases ($|\gamma_\alpha| > 1$) by factor $|\gamma_\alpha|$ per period. In total there can be at most four $|\gamma_\alpha| < 1$ and four $|\gamma_\alpha| > 1$, see Appendix A. The modes with $|\gamma_\alpha| < 1$ will be called D modes (decaying modes) and labeled by $\alpha = 1, 2, \ldots$

If $\gamma_\alpha = e^{i\theta_\alpha}$, where θ_α is a purely real phase, then the partial mode α of type (1) acquires only the phase shift by θ_α after having passed the unit cell. Hence, such Bloch modes are characterized by purely real Bloch wave numbers $k_\alpha = \theta_\alpha/l$ and propagate freely across the phononic crystal, like bulk waves in a homogeneous medium, so we will call them B modes. They occur in pairs of modes of which the energy fluxes have opposite directions along the normal to the layers. We will assign the subscripts i_m (incident) and r_m (reflected) to the modes of the m^{th} pair with understanding that the modes i_m and r_m, respectively, carry the energy towards the surface and towards interior of the half-infinite structure (see Appendix A). There can be up to four pairs of B modes in an allowed zone, i.e., the index m can be $m = 1, 2, 3,$ or 4.

III. BOUNDARY CONDITIONS

We assume that outside the phononic crystals is a free space (vacuum). In this case wave (1) is accompanied by a wave of electric potential $\varphi_v(\mathbf{r},t) = d_v e^{kz+i[kx-\omega t]}$ in the free external space ($z < 0$), where d_v is a complex amplitude and $x = \mathbf{mr}$. The direction of propagation is the axis X (Fig. 1).

A surface wave is sought for in the phononic crystal as a linear combination of D modes $\boldsymbol{\xi}_\alpha(z) = \hat{\mathbf{M}}_z(z)\boldsymbol{\zeta}_\alpha$,

$$\boldsymbol{\xi}_{\text{saw}}(z) = \sum_{\alpha=1}^{4-n} b_\alpha\boldsymbol{\xi}_\alpha(z) = \hat{\mathbf{M}}_z(z)\sum_{\alpha=1}^{4-n} b_\alpha\boldsymbol{\zeta}_\alpha, \tag{7}$$

where n is the number of pairs of B modes. The coefficients b_α are determined from the boundary conditions at $z = 0$ which are written in terms of the components of the vector $\boldsymbol{\xi}_{\text{saw}}(0) = \sum_{\alpha=1}^{4-n} b_\alpha\boldsymbol{\zeta}_\alpha$. If the phononic crystal is formed of homogeneous layers then, in the general case, $\boldsymbol{\xi}_{\text{saw}}(z)$ in the jth layer is a linear combination of the eight partial solutions

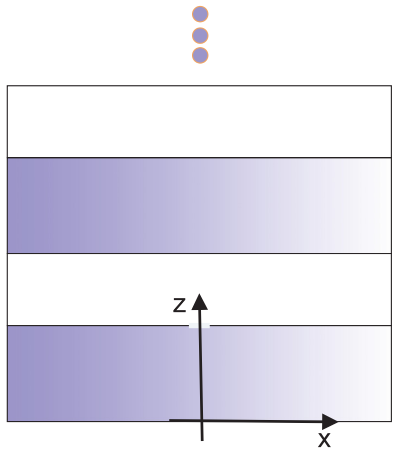

FIG. 1. Geometry of propagation. As an example, the phononic crystal composed of two alternating layers is depicted. The half-space $z < 0$ is the vacuum.

$\boldsymbol{\xi}_\alpha^{(j)} e^{i p_\alpha^{(j)} z}$ of (2), where $\boldsymbol{\xi}_\alpha^{(j)}$ and $p_\alpha^{(j)}$, $\alpha = 1, \dots, 8$, are the eigenvectors and eigenvalues of the matrix $\hat{\mathbf{N}}_j$. In consequence, in layers $\boldsymbol{\xi}_{\text{saw}}(z)$ changes with z in an involved way but on the period boundaries $z_n = nl$ one has $\boldsymbol{\xi}_{\text{saw}}(z_n) = \sum_\alpha b_\alpha \gamma_\alpha^n \boldsymbol{\zeta}_\alpha$, so the global trend of the z-dependence is $\boldsymbol{\xi}_{\text{saw}}(z) \propto |\gamma|^{z/l}$, i.e., $\boldsymbol{\xi}_{\text{saw}}(z)$ tends to zero as $|\gamma|^{z/l} \equiv e^{-\text{Im}(k_b)z}$ with increasing z, where $|\gamma| \equiv |e^{ik_b l}| = max(|\gamma_\alpha|) < 1$ and k_b is a complex Bloch wave number with $\text{Im}(k_b) > 0$.

A BIC-SAW may involve at most three D modes or two D modes or one D-mode in a phononic crystal within the frequency interval where one pair of B modes exists or two or three pairs of B modes exist, respectively. We will use the notation BIC-SAW1, BIC-SAW2 and BIC-SAW3, where the digit is the number of pairs of B modes coexisting with the BIC-SAW.

The boundary conditions at $z = 0$ require the vanishing of the traction and the continuity of the potential and z component of the electric displacement. Thus the peculiarity of the BIC-SAW problem is in the fact that there are less localized modes to form BIC-SAWs than the number of boundary conditions. In the present case, there are five boundary conditions whereas a BIC-SAW may involve at most four modes, namely, $\varphi_v(\mathrm{r}, t)$ and not more than three D modes in the phononic crystal. As a consequence of this peculiarity, BIC-SAWs are determined by several equations. When analyzing systems of equations, we will use the implicit function theorem [46]. The essence of this theorem is as follows. Suppose that m functions $f_i(\boldsymbol{\tau})$, $i = 1, \dots, m$, of $m + n$ variables $\boldsymbol{\tau} = \tau_1, \dots, \tau_{m+n}$ vanish at the point $\boldsymbol{\tau}_0 = \tau_{1,0}, \dots, \tau_{m+n,0}$. Suppose that the Jacobian, i.e., the determinant J of the $m \times m$ matrix with elements $J_{ij} = \partial f_j / \partial \tau_i$, $i, j = 1, \dots, m$, is different from zero at τ_0. In this case the system $f_i(\boldsymbol{\tau}) = 0$, $i = 1, \dots, m$, allows m variables $\tau_1, \dots, \tau_m$ to be found as functions of $\tau_{m+1}, \dots, \tau_{m+n}$ in the vicinity of $\boldsymbol{\tau}_0$. In other words, one can assert that the system $f_i(\boldsymbol{\tau}) = 0$, $i = 1, \dots, m$, yields m conditions on $m + n$ variables τ provided that $J \neq 0$. When $J = 0$, the solutions does not need to exist for $\boldsymbol{\tau} \neq \boldsymbol{\tau}_0$, so one cannot make a definite conclusion regarding the actual number of conditions.

In what follows, we will write the boundary conditions in terms of five component vectors

$$\mathbf{S}_\alpha = \begin{pmatrix} \mathbf{V}_\alpha \\ \Phi_\alpha \end{pmatrix}, \quad \mathbf{S}_v = \begin{pmatrix} \mathbf{0} \\ -i\varepsilon_0 k \\ 1 \end{pmatrix}. \tag{8}$$

The vectors $\mathbf{S}_\alpha$, $\alpha \neq v$, are formed of the components of vectors $\boldsymbol{\zeta}_\alpha$. The components of these vectors have the same meaning as those of the vector $\boldsymbol{\xi}$ (3) but we use somewhat different notation,

$$\boldsymbol{\zeta}_\alpha = \begin{pmatrix} \mathbf{U}_\alpha \\ \mathbf{V}_\alpha \end{pmatrix}, \quad \mathbf{U}_\alpha = \begin{pmatrix} \mathbf{A}_\alpha \\ \Phi_\alpha \end{pmatrix}, \quad \mathbf{V}_\alpha = \begin{pmatrix} \mathbf{L}_\alpha \\ \mathrm{D}_\alpha \end{pmatrix}. \tag{9}$$

The vector $\mathbf{S}_v$ characterizes the mode $\varphi_v(\mathbf{r}, t)$. Its first three components (traction) $\mathbf{0}$ are zeros, the fourth component is the z component of the electric displacement produced at $z = 0$ by unit potential (fifth component) times the imaginary unity. Introducing $\mathbf{S}_v$ we take into account the definition of D_α in (9).

The symbols $\boldsymbol{\tau} = \tau_1, \dots, \tau_n$ and $\boldsymbol{\tau}_0 = \tau_{1,0}, \dots, \tau_{n,0}$ will denote, respectively, the set of parameters specifying the conditions of wave propagation and a root of the system of equations under consideration. By parameters we mean frequency, wave number k, orientation angles, etc.

IV. BIC-SAWS AND LEAKY SAWS

In a frequency interval where n pairs of B modes exist a leaky SAW (pseudo-SAW or else quasi-BIC-SAW) may involve n modes carrying the energy towards the interior of the substrate, i.e., n modes labeled by the subscripts r_m, $m = 1, \dots, n$, and $4 - n$ D modes. Correspondingly, this wave is sought for in the phononic crystal as a linear combination

$$\boldsymbol{\xi}_{lsaw}(z) = \sum_{\alpha=1}^{4-n} d_\alpha \boldsymbol{\xi}_\alpha(z) + \sum_{m=1}^{n} d_{r_m} \boldsymbol{\xi}_{r_m}(z) \tag{10}$$

of partial modes $\boldsymbol{\xi}_\beta(z) = \hat{\mathbf{M}}_z(z)\boldsymbol{\zeta}_\beta$ (cf: (7)). The coefficients d_β are determined from the boundary conditions on the external surface which yield the equality

$$\sum_{\alpha=1}^{4-n} d_\alpha \mathbf{S}_\alpha + \sum_{m=1}^{n} d_{r_m} \mathbf{S}_{r_m} = d_v \mathbf{S}_v, \tag{11}$$

where at least one of d_{r_m}, $m = 1, \dots, n$, does not vanish.

At first glance, it is natural to analyze the existence of BIC-SAWs starting from the dispersion equation for leaky SAWs. However this way does not yield results. As an example, we consider BIC-SAW1s.

In the presence of one pair of B modes, (11) reduces to

$$\sum_{\alpha=1}^{3} d_\alpha \mathbf{S}_\alpha + d_{r_1} \mathbf{S}_{r_1} = d_v \mathbf{S}_v, \quad d_{r_1} \neq 0, \tag{12}$$

and a leaky SAW turns into a BIC-SAW1 if $d_{r_1} = 0$, i.e., if the B-mode is excluded. By combining the fourth and fifth lines in (12) we write this equality in the form $\hat{\mathbf{Z}}_{r\varepsilon}\mathbf{U} = 0$, where $\mathbf{U} = \sum_{\alpha=1}^{3} b_\alpha \mathbf{U}_\alpha + b_{r_1} \mathbf{U}_{r_1}$,

$$\hat{\mathbf{Z}}_{r\varepsilon} = \hat{\mathbf{Z}}_r - \varepsilon_0 k \hat{\mathbf{I}}''. \tag{13}$$

In (13), $\hat{\mathbf{Z}}_r$ is the 4×4 matrix which expresses the vectors $\mathbf{V}_\alpha$ in terms of $\mathbf{U}_\alpha$, $\alpha = r_1, 1, 2, 3$, namely, $\mathbf{V}_\alpha = -i\hat{\mathbf{Z}}_r\mathbf{U}_\alpha$, so $\hat{\mathbf{Z}}_r = i\hat{\mathbf{V}}\hat{\mathbf{U}}^{-1}$, where $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ are 4×4 matrices of which the columns are the vectors $\mathbf{U}_\alpha$ and $\mathbf{V}_\alpha$, $\alpha = r_1, 1, 2, 3$, respectively, and $\hat{\mathbf{U}}^{-1}$ is the inverse matrix $\hat{\mathbf{U}}$. The 4×4 matrix $\hat{\mathbf{I}}''$ has the single nonzero element $I''_{44} = 1$.

Solutions of (12) occur at frequencies fulfilling the equation $\det\hat{\mathbf{Z}}_{r\varepsilon} = 0$. By taking into account (8) and (9), $\det\hat{\mathbf{Z}}_{r\varepsilon}$ can be cast into the form

$$\det\hat{\mathbf{Z}}_{r\varepsilon} = \frac{\det\hat{\mathbf{B}}_\varepsilon}{\det\hat{\mathbf{U}}},\quad \hat{\mathbf{B}}_\varepsilon = \mathbf{S}_{r_1 123 v}. \tag{14}$$

Here and below the symbol $\mathbf{S}_{ijklm}$ stands for the 5×5 matrix of which the columns are the vectors $\mathbf{S}_\alpha$, $\alpha = i, j, k, l, m$, ordered in accordance with the order of subscripts in $\mathbf{S}_{ijklm}$, e.g., $\mathbf{S}_{r_1}$ and $\mathbf{S}_1$ are the first and second columns, respectively, of $\mathbf{S}_{r_1 123 v}$.

In the presence of B modes, $\hat{\mathbf{Z}}_{r\varepsilon}$ is a non-Hermitian matrix, so $\det\hat{\mathbf{Z}}_{r\varepsilon}$ is a complex valued function and usually $\det\hat{\mathbf{Z}}_{r\varepsilon} = 0$ has complex roots $\omega_c = \omega - i\omega'$ specifying leaky SAW frequencies. When the root is purely real, i.e., $\omega' = 0$ and hence there are no losses, one obtains a BIC-SAW, since if (12) holds true for purely real frequencies then from the law of the energy conservation it follows that $d_{r_1} = 0$. [Formally $d_{r_1} = 0$ at $\omega' = 0$ can be proved by using (A6)–(A9).]

The purely real parameters determining the existence of BIC-SAW1s have to satisfy the system of two equations

$$\mathrm{Re}(\det\hat{\mathbf{Z}}_{r\varepsilon}) = \mathrm{Im}(\det\hat{\mathbf{Z}}_{r\varepsilon}) = 0 \tag{15}$$

but its Jacobian necessarily vanishes since by (B5)

$$\frac{\partial \det\hat{\mathbf{Z}}_{r\varepsilon}}{\partial\tau_j} = aQ_j,\quad j = 1, 2, \ldots, \tag{16}$$

where Q_j is a purely real quantity and the factor a is the same for all the derivatives, so the rows of the Jacobian are linearly dependent. Hence we cannot establish the number of conditions for the existence of BIC-SAW1s. The same is valid for BIC-SAW2s and BIC-SAW3s.

Note that (15) is equivalent to the equality $\omega' = 0$. Since $\omega'(\boldsymbol{\tau})$ cannot change sign, it is unclear if in the general case $\omega' = 0$ only at secluded points $\boldsymbol{\tau}_0$ or there is a continuous set of points at which $\omega' = 0$. The results obtained below reveal that ω' vanishes on continuous subsets of the parameter set $\boldsymbol{\tau}$.

V. BIC-SAWS IN THE CASE OF GENERIC CRYSTALLOGRAPHIC SYMMETRY

A suitable system of equations may be derived as follows. Let a linear combination involving n pairs of B modes and $4-n$ D modes be such that for each of the pairs of B modes the amplitudes of the modes r_m and i_m, $m = 1, \ldots, n$, are equal. This linear combination satisfies the boundary conditions when

$$\sum_{\alpha=1}^{4-n} b_\alpha\mathbf{S}_\alpha + \sum_{m=1}^{n} b_{q_m}\mathbf{S}_{q_m} = d_v\mathbf{S}_v, \tag{17}$$

where $\mathbf{S}_{q_m} = \mathbf{S}_{i_m} + \mathbf{S}_{r_m}$ [cf. (11)]. By combining the fourth and fifth rows we bring (17) into the form

$$\hat{\mathbf{Z}}_{q\varepsilon}\mathbf{U} = 0,\quad \hat{\mathbf{Z}}_{q\varepsilon} = \hat{\mathbf{Z}}_q - \varepsilon_0 k\hat{\mathbf{I}}'', \tag{18}$$

where $\mathbf{U} = \sum_{\alpha=1}^{4-n} b_\alpha\mathbf{U}_\alpha + \sum_{m=1}^{n} b_{q_m}\mathbf{U}_{q_m}$, $\mathbf{U}_{q_m} = \mathbf{U}_{i_m} + \mathbf{U}_{r_m}$. The matrix $\hat{\mathbf{Z}}_q$ is defined by the relations $\mathbf{V}_\alpha = -i\hat{\mathbf{Z}}_q\mathbf{U}_\alpha$, $\alpha = q_1, 1, 2, 3$, or $\alpha = q_1, q_2, 1, 2$, or $\alpha = q_1, q_2, q_3, 1$, and $\mathbf{V}_{q_m} = \mathbf{V}_{i_m} + \mathbf{V}_{r_m}$. Hence $\hat{\mathbf{Z}}_q = i\hat{\mathbf{V}}\hat{\mathbf{U}}^{-1}$, where $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ are the 4×4 matrices of which the columns ar the vectors $\mathbf{U}_\alpha$ and $\mathbf{V}_\alpha$, labelled by the above subscripts.

Further, we introduce the vector

$$\boldsymbol{\zeta}_s \equiv \begin{pmatrix}\mathbf{U}_s\\ \mathbf{V}_s\end{pmatrix} = \sum_{\alpha=1}^{4-n} b_\alpha\boldsymbol{\zeta}_\alpha + \sum_{m=1}^{n} b_{q_m}\boldsymbol{\zeta}_{q_m}, \tag{19}$$

where $\boldsymbol{\zeta}_{q_m} = \boldsymbol{\zeta}_{i_m} + \boldsymbol{\zeta}_{r_m}$. By virtue of (A6)–(A9) for arbitrary values of b_α and b_{q_m},

$$\boldsymbol{\zeta}_s^\dagger\hat{\mathbf{T}}\boldsymbol{\zeta}_s = \mathbf{U}_s^\dagger\mathbf{V}_s + \mathbf{V}_s^\dagger\mathbf{U}_s = i\mathbf{U}_s^\dagger(\hat{\mathbf{Z}}_q^\dagger - \hat{\mathbf{Z}}_q)\mathbf{U}_s = 0, \tag{20}$$

wherefrom it follows that $\hat{\mathbf{Z}}_q$ and hence $\hat{\mathbf{Z}}_{q\varepsilon}$ are Hermitian matrices because $\mathbf{U}_s$ is an arbitrary vector [cf. $\hat{\mathbf{Z}}_{r\varepsilon}$ (13)]. Therefore $\det\hat{\mathbf{Z}}_{q\varepsilon}$ is a purely real function, so (17) holds true if the single condition $\det\hat{\mathbf{Z}}_{q\varepsilon} = 0$ is satisfied. A BIC-SAWn ($n = 1, 2, 3$) exists provided that all the coefficients b_{q_m}, $m = 1, \ldots, n$, vanish. In the general case, b_{q_m}'s are complex valued functions.

A. BIC-SAW1

In (17) $n = 1$, so the variables τ_j, $j = 1, 2, \ldots$, have to fulfill three equalities:

$$\det\hat{\mathbf{Z}}_{q\varepsilon} = 0,\quad \mathrm{Re}(b_{q_1}) = 0,\quad \mathrm{Im}(b_{q_1}) = 0. \tag{21}$$

Let us write $\det\hat{\mathbf{Z}}_{q\varepsilon}$ and b_{q_1} in the form

$$\det\hat{\mathbf{Z}}_{q\varepsilon} = \frac{\det\hat{\mathbf{B}}_{q\varepsilon}}{\det\hat{\mathbf{U}}},\quad \hat{\mathbf{B}}_{q\varepsilon} = \mathbf{S}_{q_1 123 v},$$
$$b_{q_1} = \frac{1}{2}\det\hat{\mathbf{B}}_q^*,\quad \hat{\mathbf{B}}_q = \mathbf{S}_{q_1 12 v q_1'}. \tag{22}$$

$\hat{\mathbf{B}}_q^*$ is the complex conjugate matrix $\hat{\mathbf{B}}_q$ of which the last columns is $\mathbf{S}_{q_1'} = \mathbf{S}_{i_1} - \mathbf{S}_{r_1}$. The expression of $\det\hat{\mathbf{Z}}_{q\varepsilon}$ follows from the definition of $\hat{\mathbf{Z}}_{q\varepsilon}$ and of the vectors $\mathbf{U}_\alpha$, $\mathbf{V}_\alpha$, and $\mathbf{S}_\alpha$. To derive expression (22) for b_{q_1} we insert $\mathbf{S}_{i_1} = (\mathbf{S}_{q_1} + \mathbf{S}_{q_1'})/2$ and $\mathbf{S}_{r_1} = (\mathbf{S}_{q_1} - \mathbf{S}_{q_1'})/2$ in (B1) and multiply the resulting identity from the right by the vector $\mathbf{S}$ with components $S_i = \epsilon_{ijklm}S^*_{q_1,j}S^*_{1,k}S^*_{2,l}S^*_{v,m}$. This yields

$$\sum_{\alpha=1}^{3} b_\alpha\mathbf{S}_\alpha + b_7\mathbf{S}_7 + b_{q_1}\mathbf{S}_{q_1} = d_v\mathbf{S}_v, \tag{23}$$

where b_{q_1} is given by (22),

$$b_\alpha = \det\hat{\mathbf{B}}_\alpha^*,\quad \hat{\mathbf{B}}_\alpha = \mathbf{S}_{q_1 12 v\beta},\quad \alpha = 1, 2, 3,$$
$$b_7 = -\det\hat{\mathbf{B}}_{q\varepsilon}^*,\quad d_v = -\frac{\det\hat{\mathbf{B}}_v}{2i\varepsilon_0 k},\quad \hat{\mathbf{B}}_v = \mathbf{S}_{q_1 12 v v^*}, \tag{24}$$

the last column in $\hat{\mathbf{B}}_\alpha$, $\alpha = 1, 2, 3$, is the vector $\mathbf{S}_\beta$, $\beta = \alpha + 4$, and v^* in $\mathbf{S}_{q_1 12 v v^*}$ means that the last column is $\mathbf{S}_v^*$. If $\det\hat{\mathbf{Z}}_{q\varepsilon} = 0$ then, due to the expression of $\det\hat{\mathbf{Z}}_{q\varepsilon}$ given in (22), $b_7 = 0$ and (23) reduces to (17) with $m = 1$. [In deriving the above expressions it was assumed that $\mathbf{S} \neq 0$. The vector $\mathbf{S}$ vanishes when the four five component vectors

$\mathbf{S}_\alpha$, $\alpha = q_1, 1, 2, v$, are linearly dependent. This may happen at certain particular values of parameters rather than in the general case.]

Suppose that system (21) has a root $\boldsymbol{\tau}_0$. The derivatives of $\det \hat{\mathbf{Z}}_{q\varepsilon}$ and b_{q1} at τ_0 are given in Appendix C. They are calculated in a way similar to that described in Appendix B. The Jacobian $J_{\tau_1\tau_2\tau_3}$ of (21) is constructed from these derivatives with respect to three variables τ_1, τ_2 and τ_3. Our examination of $J_{\tau_1\tau_2\tau_3}$ did not reveal any fundamental reason why $J_{\tau_1\tau_2\tau_3}$ must be equal to zero, such as rows or columns being always linearly dependent or all elements of a row or a column being necessarily zero [cf. $J_{\tau_1\tau_2}$ of (15)]. Hence we can conclude that $J_{\tau_1\tau_2\tau_2}$ does not vanish unless some additional conditions are imposed, e.g., on material constants. Correspondingly, the implicit function theorem allows us to conclude that in the general case three conditions has to be fulfilled for a BIC-SAW1 to occur, so, when searching for BIC-SAW1s, one has to have three free parameters which will be found as functions of a fourth one. This conclusion is supported by computations presented in Sec. VII. They confirm that $J_{\tau_1\tau_2\tau_3} \neq 0$. With $J_{\tau_1\tau_2\tau_3} \neq 0$, the system of equations (21) is solvable in the vicinity of point $\boldsymbol{\tau}_0$ and determines three functions $\tau_i(\tau_4)$, $i = 1, 2, 3$, specifying branches of BIC-SAW1s.

B. BIC-SAW2 and BIC-SAW3

In the case of BIC-SAW2, we have five equations,

$$\det \hat{\mathbf{Z}}_{q\varepsilon} = 0, \quad \mathrm{Re}(b_{q_m}) = 0, \quad \mathrm{Im}(b_{q_m}) = 0, \tag{25}$$

where $m = 1, 2$,

$$\det \hat{\mathbf{Z}}_{q\varepsilon} = \frac{\det \hat{\mathbf{B}}_{q\varepsilon}}{\det \hat{\mathbf{U}}}, \quad b_{q_m} = \frac{1}{2} \det \hat{\mathbf{B}}^*_{qm},$$
$$\hat{\mathbf{B}}_{q\varepsilon} = \mathbf{S}_{q_1 q_2 12 v}, \quad \hat{\mathbf{B}}_{qm} = \mathbf{S}_{q_1 q_2 1 v q'_m}, \quad m = 1, 2, \tag{26}$$

the last column of $\hat{\mathbf{B}}_{qm}$ is $\mathbf{S}_{q'_m} = \mathbf{S}_{i_m} - \mathbf{S}_{r_m}$. Expressions (26) are derived similarly to (B3) and (22).

Suppose that five equalities (25) holds true at the point $\boldsymbol{\tau}_0$. The Jacobian $J_{\tau_1 \ldots \tau_5}$ is constructed from the derivatives of $\det \hat{\mathbf{Z}}_{q\varepsilon}$ and b_{qm} with respect to five variables τ_j, $j = 1, \ldots, 5$. These derivatives are given in Appendix C. The examination of $J_{\tau_1 \ldots \tau_5}$ reveals that $J_{\tau_1 \ldots \tau_5}$, similar to $J_{\tau_1\tau_2\tau_3}$, does not vanishes unless some additional special conditions are obeyed. Therefore, by the implicit function theorem in the general case five conditions have to be satisfied for a BIC-SAW2 to exist. Numerical computations confirm this fact (Sec. VII).

As applied to BIC-SAW3, system (25) involves seven equations ($m = 1, 2, 3$) and by referring to the implicit function theorem we deduce that generally seven conditions must be fulfilled for a BIC-SAW3 to emerge. However, we cannot confirm this conclusion by numerical computations (see the discussion in Sec. VIII).

VI. CRYSTALLOGRAPHIC SYMMETRY

The crystallographic symmetry may reduce the number of conditions for the existence of BIC-SAWs. Assume that either all the layers have the plane of symmetry ("P") or all the layers have the two-fold symmetry axis ("**2**"). In addition, let all the layers be oriented identically in such a way that the vectors **n** and **m**, which specify the geometry of propagation of wave (1), are oriented in accordance with one of the following four options.

$$(1)\ \mathbf{n}\perp \mathrm{P}, \quad (2)\ \mathbf{n}\parallel \mathbf{2}, \quad (3)\ \mathbf{m}\perp \mathrm{P}, \quad \text{and}\ (4)\ \mathbf{m}\parallel \mathbf{2}. \tag{27}$$

It is worth noting that for these orientations, excluding orientations fulfilling additional conditions, the D and B modes have all the components of the mechanical displacement and traction and are piezoactive. Therefore the boundary conditions on the external surface mix the D and B modes, so, despite the symmetry, it is not obvious that BIC-SAWs can arise in these cases.

When the structure assumes orientations (27), the eigenvectors of the transfer matrix possess specific properties, see (D6)–(D8). From (D6) and the equality $\hat{\mathbf{K}}^2 = 1$ it follows that $\boldsymbol{\zeta}^*_{q_n} = \hat{\mathbf{K}}\boldsymbol{\zeta}_{q_n}$ and $\boldsymbol{\zeta}^*_{q'_n} = -\hat{\mathbf{K}}\boldsymbol{\zeta}_{q'_n}$, where $\boldsymbol{\zeta}_{q'_n} = \boldsymbol{\zeta}_{i_n} - \boldsymbol{\zeta}_{r_n}$. Therefore, in view of (D3) and (D4),

$$\mathbf{S}^*_{q_n} = \hat{\mathbf{\Delta}}_s \mathbf{S}_{q_n}, \quad \mathbf{S}^*_{q'_n} = -\hat{\mathbf{\Delta}}_s \mathbf{S}_{q'_n}, \quad \hat{\mathbf{\Delta}}_s = \begin{pmatrix} \hat{\mathbf{\Delta}} & \hat{\mathbf{0}}' \\ \hat{\mathbf{0}}'^t & -1 \end{pmatrix}, \tag{28}$$

where $\hat{\mathbf{\Delta}}_s$ is a 5×5 matrix, $\hat{\mathbf{\Delta}}$ is the 4×4 matrix (D3) and the symbol $\hat{\mathbf{0}}'$ stands for the 4×1 column of zeros. The S-vectors of D modes obey the relations

$$\mathbf{S}^*_\beta = \hat{\mathbf{\Delta}}_s \mathbf{S}_\alpha, \tag{29}$$

where the modes α and β correspond to the complex conjugate eigenvalues $\gamma^*_\alpha = \gamma_\beta$. If γ_α is purely real then α and β label the same mode, i.e., $\beta = \alpha$ in (29).

Substituting (28) and (29) in the matrix $\hat{\mathbf{B}}^*_q$ (22) yields

$$b_{q_1} = \pm\tfrac{1}{2} \det(\hat{\mathbf{\Delta}}_s \hat{\mathbf{B}}_q) = \mp\tfrac{1}{2} \det \hat{\mathbf{B}}_q = \mp b^*_{q_1}, \tag{30}$$

the sign $\pm$ indicates that the insertion of (29) can change the sequence of columns in the matrix.

Thus b_{q_1} is either a purely real or purely imaginary function and hence two equations, rather than three (21), condition the existence of BIC-SAW1s,

$$\det \hat{\mathbf{Z}}_{q\varepsilon} = 0, \quad b_{q_1} = 0. \tag{31}$$

By analogy, equations (25) simplify to

$$\det \hat{\mathbf{Z}}_{q\varepsilon} = 0, \quad b_{q_m} = 0, \quad m = 1, 2, \ \text{or}\ m = 1, 2, 3, \tag{32}$$

where b_{q_m} are either purely real or purely imaginary functions, that is, the number of equations for BIC-SAW2 and BIC-SAW3 turns out to be three and four rather than, respectively, five and seven as it is in the case of arbitrary geometry of propagation.

We find that the Jacobians of (31) and (32) generally does not equal zero, so by referring to the implicit function theorem we conclude that two, three and five conditions must be met, respectively, for the existence of BIC-SAW1s, BIC-SAW2s, and BIC-SAW3s with orientations (27).

VII. NUMERICAL EXAMPLES

This section presents the results of numerical computations confirming our conclusions regarding BIC-SAWs. Namely, there are two and three conditions for the existence of a BIC-SAW1 at orientations (27) and in the general case, respectively. There are three and five conditions for the existence of a BIC-SAW2 at orientations (27) and in the general case, respectively.

It turns out that the equations derived in the previous sections allow the establishment of the number of conditions for the existence of BIC-SAWs but they are not convenient for numerical search of BIC-SAW branches. An alternative way is to search for BIC-SAWs via searching for leaky SAWs with vanishing imaginary part ω', i.e., via equations

$$\det \hat{\mathbf{Z}}_{r\varepsilon} = 0, \quad \omega' = 0. \tag{33}$$

This way proves to be technically convenient.

The impedance $\hat{\mathbf{Z}}_{r\varepsilon}$ for BIC-SAW1s is given in (13). In the case of BIC-SAW2s $\hat{\mathbf{Z}}_{r\varepsilon}$ reads similarly but the impedance $\hat{\mathbf{Z}}_r$ is expressed in terms of the matrices $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ of which the columns are the vectors $\mathbf{U}_\alpha$ and $\mathbf{V}_\alpha$, $\alpha = r_1, r_2, 1, 2$, where the indices r_1 and r_2 label two reflected B modes.

Since ω' is of definite sign, solving (33) implies finding complex roots $\omega_c = \omega - i\omega'$ of $\det \hat{\mathbf{Z}}_{r\varepsilon} = 0$ and searching for global minima $\omega' = 0$ by varying an appropriate number of parameters. The required number of variable parameters has been established in Secs. V and VI.

We always check that found SAWs are in fact BIC-SAWs. The point is that solutions of (33) may converge to SAWs in the domain where B modes are absent. Note that in certain cases it is worth using the solution of equations from Sec. IV or V found in the linear approximation as the initial guess point for equations (33) when computing BIC-SAW branches in the vicinity of a known solution in order to improve the convergence of minimization. [The linear approximation for equations (33) does not exist because of the quadratic dependence of ω' on parameters in the neighborhood of $\omega' = 0$.]

A. BIC-SAW1

We consider a 1D phononic crystals formed of alternating GaSb and InAs layers. It is supposed that the structure is grown in the [001] direction of GaSb and InAs single crystals of which the symmetry group is $\bar{4}3m$. Correspondingly the layers are piezoelectrics, the boundary is the (001) plane and the normal $\mathbf{n}$ is parallel to the rotation-inversion axis $\bar{4}$. Therefore the geometry of propagation corresponds to case 2 in (27) because the axis $\bar{4}$ includes the axis 2. We denote by GaSb/InAs and InAs/GaSb a half-infinite phononic crystal where the exterior layer is GaSb and InAs, respectively, and assume that the GaSb and InAs layers are of equal thickness h. The material constants are taken from site [47].

We will search for BIC-SAW1s by solving equations (33). In accordance with Sec. V, the complex frequency ω_c is to be found from the first equation as a function of one variable parameters in parallel with minimizing ω' by varying this parameter.

Let us vary the angle α which specifies the propagation direction on the surface and is counted off of the [100] direction. By solving the fist equation in (33) we find leaky SAWs. Figure 2 shows the leaky SAW branches (curves I and II) on InAs/GaSb and GaSb/InAs in a zone where a pair of B modes exists. Curves I and II represent the dependence of the dimensionless parameter $\omega H/v_0$ on the angle α for $kH = 2$,

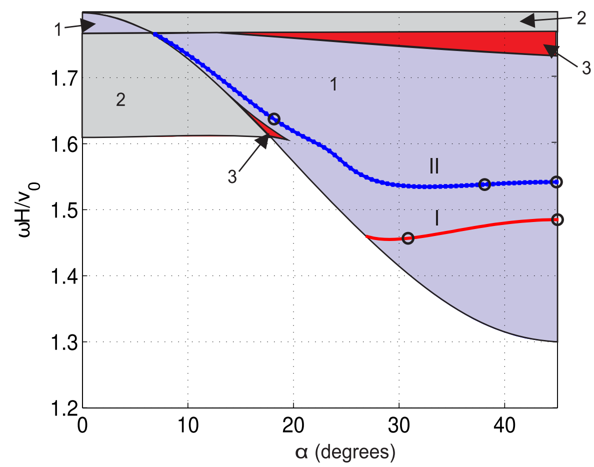

FIG. 2. Branches of leaky waves in InAs/GaSb (curve I) and GaSb/InAs (curve II) on the (001) surface for $kH = 2$. The right-hand border is $\alpha = 45^\circ$. Circles on curves I and II mark BIC-SAW1s. Digits 1,2,3 label domains where 1,2,3 pairs of B modes exist, respectively. At each point $(\alpha, \omega H/v_0)$ all the B modes have the frequency ω and wave number $k = 2/H$. There is no B modes in the blank domain.

where ω is the real part of the leaky wave frequency, $H = 2h$ is the period and the velocity v_0 is put equal to 3330 m/s.

The imaginary part of the leaky SAW frequency vanishes for the angles $\alpha \approx 18.307^\circ$ and $\alpha \approx 37.712^\circ$ in GaSb/InAs as well as for the angle $\alpha \approx 30.963^\circ$ in InAs/GaSb ($\omega'/\omega < 10^{-15}$, see Fig. 3). Hence at these angles the leaky SAW turns into the BIC-SAW1 since, as it has already been mentioned in Sec. IV, $\omega' = 0$ implies that the boundary conditions are fulfilled by a linear combination involving only D modes. The dependence of the amplitude of the BIC-SAW1, which arises at $\alpha \approx 18.307^\circ$, on the distance from the external surface of the phononic crystal is depicted in Fig. 4.

Two circles at the edge $\alpha = 45^\circ$ of Fig. 2 mark two BIC-SAW1s which can be called symmetry protected. In

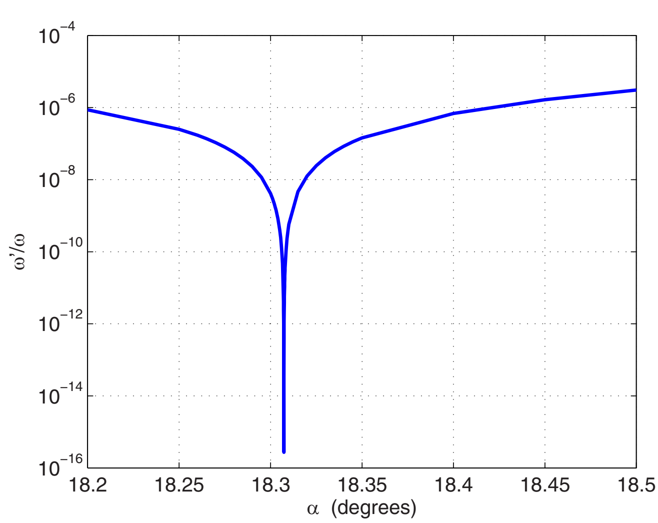

FIG. 3. Imaginary part ω' of the leaky wave frequency in the neighborhood of the angle $\alpha = 18.307^\circ$ vs α at $kH = 2$ in GaSb/InAs.

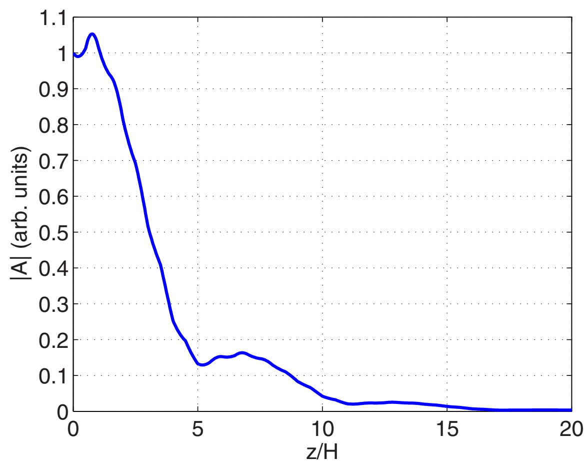

FIG. 4. Amplitude $|A| = \sqrt{\mathbf{A}^{\dagger}\mathbf{A}}$ of mechanical displacements $\mathbf{A}$ of the BIC-SAW1 existing for $\alpha = 18.307^{\circ}$ in GaSb/InAs vs the normalized distance z/H from the surface, where H is the period. Small ripples are due to changes of the wave field inside layers.

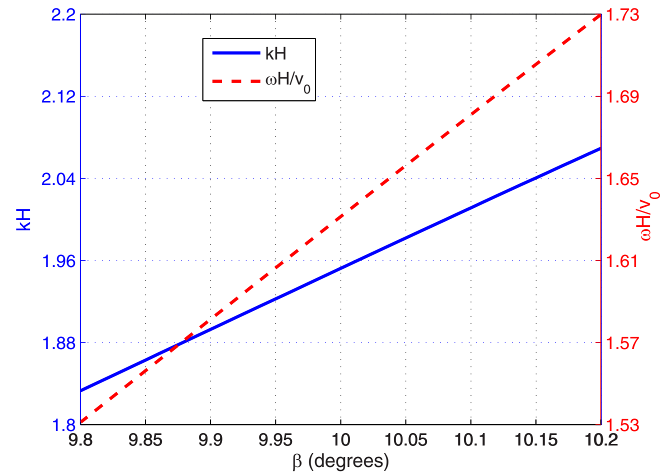

FIG. 6. The BIC-SAW1 branch in GaSb/InAs near the SAW existence point (15.667°, 10.081°, 6°), $kH = 2$ and $\omega H/v_0 = 1.671$. The β dependencies of α and kH are computed for $\gamma = 6^{\circ}$.

this case the sagittal plane is the plane of symmetry of the structure. Within domain 1 in this plane all the D modes prove to be sagittaly polarized and piezoactive whereas the B modes are shear horizontally polarized and nonpiezoactive, so the boundary conditions just cannot mix D modes and B modes. Note that the D modes forming BIC-SAW1s at $\alpha \neq 45^{\circ}$ as well as the B modes in domain 1 for $\alpha \neq 0^{\circ}, 45^{\circ}$ are piezoactive and have all the three components of mechanical displacement and traction.

Calculations reveal that the Jacobian of equations (31) with respect to ω and α does not vanish at the point of the existence of BIC-SAW1 found for $\alpha \approx 18.307^{\circ}$, so a BIC-SAW1 branch may be found in the form of the dependence of ω and α on a third parameter. Figure 5 shows $\omega(k)$ and $\alpha(k)$ computed by (33) and ω' is minimized by varying α for a given k. Note that the same dependences calculated through the linear approximation of equations (31) differ hardly from lines in Fig. 5.

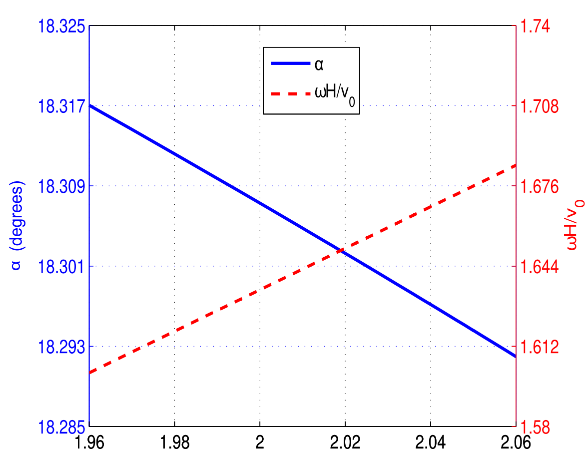

FIG. 5. The BIC-SAW1 branch in GaSb/InAs on the (001) surface in the neighborhood of the angle $\alpha = 18.307\ldots^{\circ}$ The wave number k changes in the vicinity of the value $2/H$. The angle α and the value of $\omega H/v_0$ are shown as functions of kH.

Let us consider the case of generic orientations of layers. As the initial orientation, we take the one where the vectors $\mathbf{n}$ and $\mathbf{m}$ are along the [001] and [100] directions, respectively, i.e., along the Z and X axes. The orientation of each layer is characterized by three angles α, β, and γ which specify three consequential rotations about the axes Z, the new X, and the new Y, respectively. However, in the cases considered in this section the orientation of all the layers changes identically.

In particular, the BIC-SAW1 existing on the (001) plane of the GaSb/InAs phononic crystal at the angle $\alpha \approx 18.307^{\circ}$ and $kH = 2$ (see Fig. 2) gives rise to the BIC-SAW1 branch. Note that the Jacobian $J_{\omega,kH,\alpha}$ of Eqs. (21) with respect to ω, kH and α vanishes for symmetric orientations of the type $(\alpha, 0, 0)$. At the same time, the Jacobian with respect to ω and the angles α and β is not zero. Therefore one may calculate the BIC-SAW1 branch in the form of the dependencies of ω, α and β on the angle γ for a fixed $kH = 2$ by solving equations (33) and minimizing ω' by varying α and β. When searching for BIC-SAW1s, the orientation was changed as follows. First the rotation was performed about the axis Z at the angle α, then about the new axis X at the angle β and finally about the new axis Y at the fixed angle γ.

With $\beta, \gamma \neq 0$, the Jacobian $J_{\omega,kH,\alpha}$ of equations (21) does not vanish. Accordingly, having fixed, for instance, the angle γ, it is now convenient to search for ω, kH and α as functions of the angle β. An example of such dependencies calculated by equations (33) are shown in Figs. 6 and 7. The same lines may be calculated via linear approximation of equations (21). The lines $\omega(\beta)$ and $kH(\beta)$ obtained by these two methods almost merge. The lines $\alpha(\beta)$ are slightly different, see Fig. 7.

B. BIC-SAW2

Since our aim is to confirm conclusions of Secs. V and VI regarding BIC-SAW2s, we may use InAs and a fictitious material, modified GaSb (m-GaSb), in which the elastic moduli c_{44} and c_{66} of GaSb are replaced by $c_{44} = c_{66} = 47.5$ GPa.

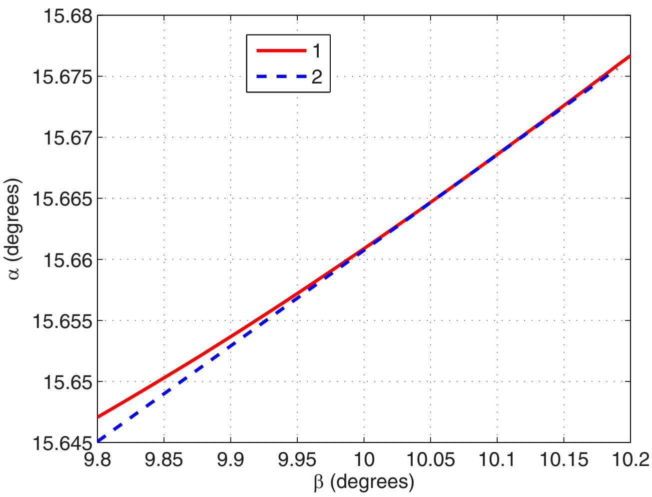

FIG. 7. Angle α vs angle β computed by equations (33), line 1, and by linear approximation of equations (21), line 2, for $\gamma = 6^\circ$.

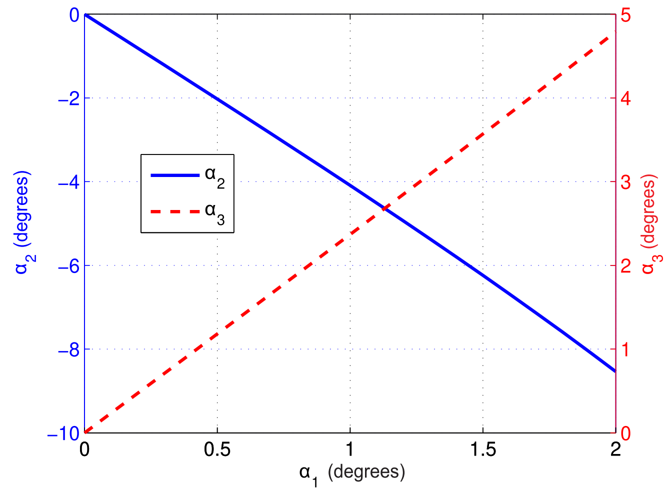

FIG. 8. Angles α_2 and α_3 specifying the BIC-SAW2 branch vs angle α_1 (angle α_4 equals zero). The orientation is of the type $\mathbf{n}\|\mathbf{2}$, $kH = 2$ and H is the sum of the thickness of only two layers.

The symmetry of m-GaSb is 222 with axes twofold symmetry axes along [100], [010], and [001] directions.

First assume that all the layers are oriented likely, [100] and [001] directions are along the axes X and Z, respectively, the axis Z is the normal to the surface. Since a change of c_{44} and c_{66} does not affect the spectrum of modes propagating and polarized in the plane XZ, in the InAs/m-GaSb phononic crystal, like in the InAs/GaSb one, in the interval of $\omega H/v_0$ from 1.61 to 1.77 there are four sagittally polarized B modes, see the spectrum in Fig. 2 for $\alpha = 0$. Around the X axis there is a zone with four B modes. It is similar to the left-most zone 2 adjusted to the X direction ($\alpha = 0$) in Fig. 2. At the same time, in contrast to InAs/GaSb, in InAs/m-GaSb a shear horizontally (SH) polarized piezoactive SAW emerges at $\omega H/v_0 = 1.685$ along the axis X. Such a BIC-SAW2 exist thanks to the separation of the modes propagating in the plane perpendicular to the axis 2 into sagittally polarized modes and SH-polarized modes. (In the XZ plane, i.e., for $\alpha = 0$, the moduli c_{44} and c_{66} affect only SH modes.)

This symmetry protected SH BIC-SAW2 helps us to find branches of BIC-SAW2s for one of the types of orientations (27), $\mathbf{n}\|\mathbf{2}$, and for general orientations in a phononic crystal with unit cell containing four layers $InAs^1$/m-$GaSb^2$/$InAs^3$/m-$GaSb^4$ of equal thickness. The superscript i numbers layers, the orientation of the ith layer is described by the angles $(\alpha_i, \beta_i, \gamma_i)$ which specify the consequential rotations about the axis Z, new axis X, and new axis Y, respectively.

Let $\beta_i = \gamma_i = 0$ and $i = 1, \ldots, 4$. With $\alpha_i \neq 0$, i.e., at rotation about the axis Z $\|\mathbf{n}\|\mathbf{2}$, the geometry of propagation is of the type $\mathbf{n}\|\mathbf{2}$. The SH BIC-SAW2 turns into the leaky SAW when, e.g., $\alpha_1 \neq 0$. According to Sec. VI, in the case $\mathbf{n}\|\mathbf{2}$ the existence of BIC-SAW2s constraints three parameters, in particular, ω, α_2 and α_3, which may be found as functions of the angle α_1 via Eqs. (33) and minimization of ω' by varying α_2 and α_3, see Figs. 8 and 9. The quadratic dependence of ω on α_1 is related to the symmetry of acoustic properties with respect to the plane XZ which is perpendicular to the symmetry axis 2, so the equivalence of the cases $\pm\alpha_1$ results in $\omega(\alpha_1) = \omega(-\alpha_1)$ and $\alpha_{2,3}(\alpha_1) = -\alpha_{2,3}(-\alpha_1)$.

Let now $\alpha_i = \beta_i = 0$, $i = 1, \ldots, 4$, $\gamma_1 = \gamma_3 = 8^\circ$, and $\gamma_2 = \gamma_4 = -8^\circ$. The SH BIC-SAW2 still exists in the plane XZ which remains perpendicular to the axis 2 (if $|\gamma_i| > 12^\circ$ then the SH SAW falls into an interval with two B modes, thereby becoming SH BIC-SAW1). When $\alpha_1 \neq 0$, the geometry of propagation proves to be of the general type and, according to Sec. V, five conditions have to be fulfilled for a BIC-SAW2 to exist. We chose ω, α_i and β_i, $i = 2, 3$, as the parameters to be determined for a given α_1 and, when solving equations (33), we minimize ω' by varying four angles, α_i and β_i, $i = 2, 3$, with $\alpha_4 = \beta_4 = 0$. The BIC-SAW2 branch obtained in the form of the dependence of ω, α_i and β_i, $i = 2, 3$, on α_1 is shown in Figs. 9–11.

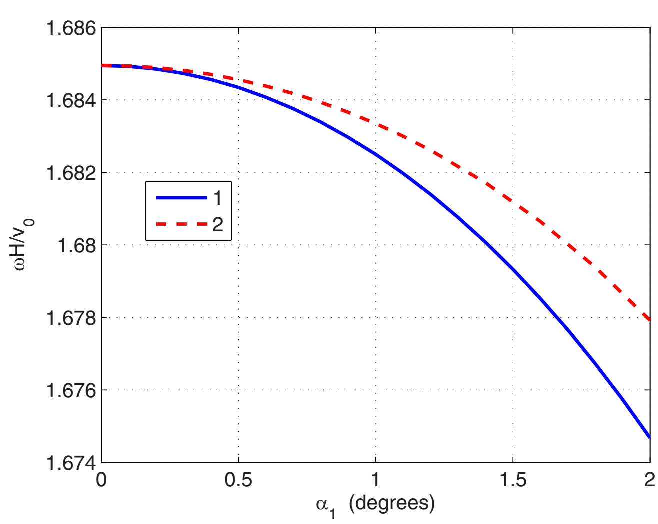

FIG. 9. BIC-SAW2 frequency vs angle α_1 for $kH = 2$, where H is the sum of the thickness of two layers. Curve 1 - BIC-SAW2 for orientation $\mathbf{n}\|\mathbf{2}$ and angle $\alpha_4 = 0$. Curve 2 - BIC-SAW2 for general orientations.

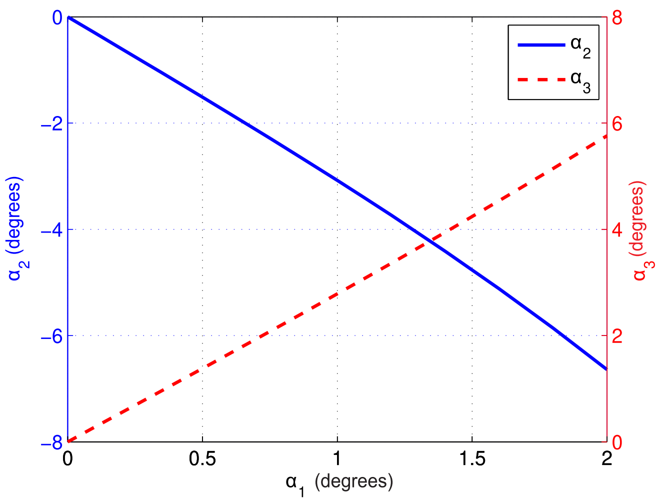

FIG. 10. Angles α_2 and α_3 specifying the BIC-SAW2 branch vs angle α_1. The orientation is of general type, $kH = 2$ and H is the sum of the thickness of only two layers.

VIII. CONCLUDING REMARKS

In this paper, the equations governing the existence of BIC-SAWs in piezoelectric 1D phononic crystals have been derived in the form which has allowed us to establish the number of conditions securing the occurrence of such SAWs. Numerical computations validate the conclusions drawn from analytic considerations. The computed branches of BIC-SAW1 and BIC-SAW2 are depicted in Figs. 5–7 and Figs. 8–11, respectively.

BIC-SAWs are robust only under consistent changes of parameters, unlike SAWs in frequency interval forbidden for B modes, i.e., for delocalized freely propagating Bloch modes. Indeed, the surface impedance in forbidden intervals proves to be a Hermitian matrix [37,38], so SAW frequencies obey a single purely real dispersion which allows one to determine the frequency as a continuous function of all the parameters

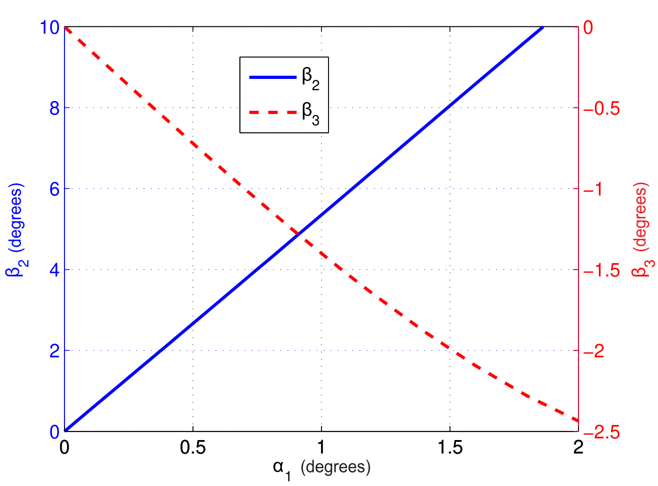

FIG. 11. Angles β_2 and β_3 specifying the BIC-SAW2 branch vs angle α_1. The orientation is of general type, $kH = 2$ and H is the sum of the thickness of only two layers.

specifying the problem. Therefore an arbitrary variation of parameters merely changes the frequency. On the contrary, according to Secs. V–VII the existence of BIC-SAWs is governed by a set of equations. In consequence, when solving the BIC-SAW problem, one finds not only the frequency but also a number of parameters as functions of the other parameters, so not all the parameters specifying the BIC-SAW propagation can be varied arbitrarily.

The number of conditions for the existence of BIC-SAWs depends on the number of B modes in a given frequency interval. In the presence of one pair of B modes, a BIC-SAW1 emerges provided that the parameters of the problem satisfy three equalities. In other words, in the general case a BIC-SAW1 is determined not only by the frequency but also by two more parameters, such as the wave number and one orientation angle specifying the geometry of propagation. The crystallographic symmetry may decrease the number of conditions to two.

The occurrence of BIC-SAW2s in the intervals where two pairs of B modes exist is more severely conditioned, since the number of decaying modes, which might form such SAWs, decreases. Five equations have to be solved to find five parameters, including frequency, for which BIC-SAW2s exist. Owing to the crystallographic symmetry the number of equations may be reduced to three.

Note that in nonpiezoelectric materials the partial solutions of system (2) split into six solutions associated with elastic modes with vanishing components corresponding to the potential and electric displacement and two solutions associated with purely electrostatic modes in which the displacement and traction components vanish. This splitting entails the similar splitting of the eigenvectors of the transfer matrix into two independent groups consisting of six eigenvectors and two eigenvectors. As a result, in accordance with definitions of vectors (8) and (9), matrices split into 3×3 diagonal blocks relevant to the SAW problem and 2×2 or 1×1 diagonal blocks formed of potentials and electric displacements of electrostatic modes which are irrelevant to the problem under consideration. For instance, this fact can be deduced from (22)–(24) assuming that with vanishing piezoeffect the modes $\alpha = 1, 5$ go to electrostatic modes and hence the first three components of the vectors $\mathbf{S}_{1,5}$ and $\mathbf{U}_{1,5}$ equal zero in this limit. Thus, the method used in the present paper allows the reproduction of the results for BIC-SAWs in nonpiezoelectric phononic crystals obtained in [44] by a different method.

Comparison with results obtained in Ref. [44] reveals that the piezoelectric effect does not entail additional conditions for the existence of BIC-SAW1s and BIC-SAW2s. In nonpiezoelectric media BIC-SAW3s cannot emerge because there is no mode to form a surface wave if there are three pairs of bulk modes. In piezoelectrics an extra acoustoelectric localized mode exists, so in principle a BIC-SAW3 is allowed. However its appearance looks to be an exceptional case not only because of the large number of constraints (seven and four in the general case and for certain symmetric orientations, respectively) but also because the piezoelectric effect must be very strong. Anyway we could not find an example of BIC-SAW3.

ACKNOWLEDGMENT

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APPENDIX A

According to Refs. [26,31],

$$\hat{\mathbf{N}} = -\begin{pmatrix} \hat{\mathbf{N}}_{11} & \hat{\mathbf{N}}_{12} \\ \hat{\mathbf{N}}_{21} & \hat{\mathbf{N}}_{11}^{t} \end{pmatrix}, \tag{A1}$$

where

$$\hat{\mathbf{N}}_{11} = k(nn)^{-1}(nm), \quad \hat{\mathbf{N}}_{12} = (nn)^{-1},$$
$$\hat{\mathbf{N}}_{21} = k^2[(mn)(nn)^{-1}(nm) - (mm)] + \rho\omega^2\hat{\mathbf{I}}', \tag{A2}$$

are the 4×4 matrices built from 4×4 matrices (ab) of which elements are contractions of the three-component vectors $\mathbf{a}$, $\mathbf{b} = \mathbf{n}$ or $\mathbf{m}$ with the material tensors of the medium, namely, $(ab)_{IJ} = a_k E_{kIJl} b_l$, $I, J = 1,\dots,4$, where $E_{kIJl} = c^E_{kIJl}$, $I, J = 1, 2, 3$, $E_{k4Jl} = e_{kJl}$, $J = 1, 2, 3$, $E_{kI4l} = e_{lIk}$, $I = 1, 2, 3$, and $E_{k44l} = -\varepsilon^S_{kl}$. The symbol $\hat{\mathbf{I}}'$ denotes the 4×4 matrix with three unit elements $I'_{ii} = 1$, $i = 1, 2, 3$, the other ones being zero.

Due to (3) the lossless condition div$\mathbf{P} = 0$ yields

$$P_z = -\boldsymbol{\xi}^{\dagger}\hat{\mathbf{T}}\boldsymbol{\xi}/4 = const, \tag{A3}$$

where P_z is the z component of the time averaged energy flux $\mathbf{P}$, the symbol † stands for Hermitian conjugation,

$$\hat{\mathbf{T}} = \begin{pmatrix} \hat{\mathbf{0}} & \hat{\mathbf{I}} \\ \hat{\mathbf{I}} & \hat{\mathbf{0}} \end{pmatrix}, \tag{A4}$$

is a 4×4 matrix formed of the zero and identity 4×4 matrices $\hat{\mathbf{0}}$ and $\hat{\mathbf{I}}$. From (2) and (A3), it follows that $(\hat{\mathbf{T}}\hat{\mathbf{N}})^{\dagger} = \hat{\mathbf{T}}\hat{\mathbf{N}}$. The same equality also follows from the explicit expression of the matrix $\hat{\mathbf{N}}$.

The transfer matrix $\hat{\mathbf{M}}$ (6) satisfies the identity

$$\hat{\mathbf{M}}^{-1} = \hat{\mathbf{T}}\hat{\mathbf{M}}^{\dagger}\hat{\mathbf{T}}, \tag{A5}$$

which follows from the relation $(\hat{\mathbf{T}}\hat{\mathbf{N}})^{\dagger} = \hat{\mathbf{T}}\hat{\mathbf{N}}$. Due to (A5) the eigensolutions $(\gamma_\alpha, \boldsymbol{\zeta}_\alpha)$, $\alpha = 1,\dots,8$ of the eigenvalue problem for the matrix $\hat{\mathbf{M}}$ occur in pairs of two types [38,48]. The first one is a pair of eigenvalues γ_α and $\gamma_{\alpha+4}$ such that $\gamma_{\alpha+4} = 1/\gamma^*_\alpha$, $|\gamma_\alpha| \neq 1$, and then the eigenvectors $\boldsymbol{\zeta}_\alpha$ and $\boldsymbol{\zeta}_{\alpha+4}$ are orthogonal to the other six eigenvectors in the sense

$$\boldsymbol{\zeta}^{\dagger}_\beta\hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha = \boldsymbol{\zeta}^{\dagger}_\beta\hat{\mathbf{T}}\boldsymbol{\zeta}_{\alpha+4} = 0, \quad \beta \neq \alpha, \alpha+4, \tag{A6}$$

but $\boldsymbol{\zeta}^{\dagger}_{\alpha+4}\hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha \neq 0$, so one can put

$$\boldsymbol{\zeta}^{\dagger}_{\alpha+4}\hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha = 1. \tag{A7}$$

The second type of eigenvalues is $\gamma_\alpha = e^{i\theta_\alpha}$ and $\gamma_{\alpha+4} = e^{i\theta_{\alpha+4}}$, where θ_α and $\theta_{\alpha+4}$ are purely real phases, so this pair corresponds to a pair of B modes. In this case, owing to (A5)

$$\boldsymbol{\zeta}^{\dagger}_\beta\hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha = \boldsymbol{\zeta}^{\dagger}_\nu\hat{\mathbf{T}}\boldsymbol{\zeta}_{\alpha+4} = 0, \quad \beta \neq \alpha, \quad \nu \neq \alpha+4, \tag{A8}$$

but $\boldsymbol{\zeta}^{\dagger}_\alpha\hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha \neq 0$ and $\boldsymbol{\zeta}^{\dagger}_{\alpha+4}\hat{\mathbf{T}}\boldsymbol{\zeta}_{\alpha+4} \neq 0$. In view of (A3) we can put

$$\boldsymbol{\zeta}^{\dagger}_{i_n}\hat{\mathbf{T}}\boldsymbol{\zeta}_{i_n} = 1, \quad \boldsymbol{\zeta}^{\dagger}_{r_n}\hat{\mathbf{T}}\boldsymbol{\zeta}_{r_n} = -1. \tag{A9}$$

Thus due to (A6)–(A9) the completeness relation of the eigenvectors of $\hat{\mathbf{M}}$ in the interval, where m pairs of B modes exist, reads as follows:

$$\sum_{\alpha=1}^{4-m}(\boldsymbol{\zeta}_\alpha \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_{\alpha+4} + \boldsymbol{\zeta}_{\alpha+4} \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_\alpha) + \sum_{n=1}^{m}(\boldsymbol{\zeta}_{i_n} \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_{i_n} - \boldsymbol{\zeta}_{r_n} \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_{r_n}) = \begin{pmatrix} \hat{\mathbf{I}} & \hat{\mathbf{0}} \\ \hat{\mathbf{0}} & \hat{\mathbf{I}} \end{pmatrix}, \tag{A10}$$

where the symbols $\otimes$ and * denote the dyadic multiplication and complex conjugation.

APPENDIX B

Let us prove (16). Suppose that (15) has a root τ_0. First, we derive expressions of the amplitudes d_α, $\alpha = 1, 2, 3, v$, of the partial modes forming the BIC-SAW1. Due to definitions (8) and (9) from (A10) it follows that

$$\sum_{\alpha=1}^{3}(\mathbf{S}_\alpha \otimes \mathbf{S}^*_{\alpha+4} + \mathbf{S}_{\alpha+4} \otimes \mathbf{S}^*_\alpha) + \mathbf{S}_{i_1} \otimes \mathbf{S}^*_{i_1} - \mathbf{S}_{r_1} \otimes \mathbf{S}^*_{r_1} = \frac{1}{2i\varepsilon_0 k}(\mathbf{S}^*_v \otimes \mathbf{S}^*_v - \mathbf{S}_v \otimes \mathbf{S}_v). \tag{B1}$$

Multiply (B1) from the right by the vector $\mathbf{S}$ with components $S_i = \epsilon_{ijklm}S^*_{r_1,j}S^*_{2,k}S^*_{3,l}S^*_{v,m}$, $i, j, k, l, m = 1,\dots,5$, where ϵ_{ijklm} is the 5×5 antisymmetric tensor, $\epsilon_{12345} = 1$, $S_{a,i}$ is the ith component of $\mathbf{S}_a$. We obtain

$$\sum_{\alpha=1}^{3} d_\alpha\mathbf{S}_\alpha + d_5\mathbf{S}_5 + d_{i_1}\mathbf{S}_{i_1} = d_v\mathbf{S}_v, \tag{B2}$$

where

$$d_\alpha = \det\hat{\mathbf{B}}^*_\alpha, \quad \hat{\mathbf{B}}_\alpha = \mathbf{S}_{r_1 23v\beta}, \quad \beta = \alpha+4,$$
$$\alpha = 1, 2, 3, \quad d_5 = -\det\hat{\mathbf{B}}^*_\varepsilon, \quad d_i = \det\hat{\mathbf{B}}^*_i, \tag{B3}$$
$$\hat{\mathbf{B}}_i = \mathbf{S}_{r_1 23vi_1}, \quad d_v = -\frac{\det\hat{\mathbf{B}}^*_v}{2i\varepsilon_0 k}, \quad \hat{\mathbf{B}}_v = \mathbf{S}_{r_1 23vv^*},$$

$\hat{\mathbf{B}}^*_j$ is the complex conjugate matrix $\hat{\mathbf{B}}_j$, the subscript v^* in $\mathbf{S}_{r_1 23vv^*}$ indicates that the last column is $\mathbf{S}^*_v$ and $\hat{\mathbf{B}}_\varepsilon$ is defined in (14).

When $\det\hat{\mathbf{Z}}_{r\varepsilon} = 0$, and hence $d_5 = 0$, for purely real parameters, d_{i_1} also vanishes because $d_{i_1} \neq 0$ would contradict the law of energy conservation. Therefore d_α, $\alpha = 1, 2, 3$, and d_v (B3) at $\boldsymbol{\tau}_0$ are the amplitudes of D modes and of the mode $\varphi_v(\mathrm{r}, t)$ which together form the BIC-SAW1.

Now let us calculate $\partial\det\hat{\mathbf{Z}}_{r\varepsilon}/\partial\tau_j$. In view of (14) $\det\hat{\mathbf{B}}_\varepsilon = 0$ at the point $\boldsymbol{\tau}_0$, so it is required to calculate $\partial\det\hat{\mathbf{B}}_\varepsilon/\partial\tau_j$ which are obtained by replacing consequently the column $\mathbf{S}_\alpha$ in $\hat{\mathbf{B}}_{q\varepsilon}$ by $\partial\mathbf{S}_\alpha/\partial\tau_j$. Due to (A6)–(A9), the latter can be represented as a linear combination of S-vectors,

$$\frac{\partial\mathbf{S}_\alpha}{\partial\tau_j} = \sum_{\beta=1}^{3}\left(\boldsymbol{\zeta}^{\dagger}_\beta\hat{\mathbf{T}}\frac{\partial\boldsymbol{\zeta}_\alpha}{\partial\tau_j}\right)\mathbf{S}_{\beta+4} + \cdots. \tag{B4}$$

After the substitution of (B4), and of $\partial\mathbf{S}_v/\partial k = (\mathbf{S}_v - \mathbf{S}^*_v)/2k$ when τ_j stands for the wave number k, some of the determinants entering $\partial\det\hat{\mathbf{B}}_\varepsilon/\partial\tau_j$ vanish because of the linear dependence of their columns. The result can be cast into the form

$$\frac{\partial \det \hat{\mathbf{Z}}_{r\varepsilon}}{\partial \tau_j} = \frac{iQ_j}{d_1 \det \hat{\mathbf{U}}}, \tag{B5}$$

where

$$\begin{aligned} Q_j &= i\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\left(\boldsymbol{\zeta}_\alpha^\dagger \hat{\mathbf{T}}\frac{\partial \boldsymbol{\zeta}_\beta}{\partial \tau_j}\right)d_\alpha^* d_\beta - \varepsilon_0|d_v|^2 \\ &= i\left(\boldsymbol{\zeta}_D^\dagger \hat{\mathbf{T}}\frac{\partial \boldsymbol{\zeta}_D}{\partial \tau_j}\right) - \varepsilon_0|d_v|^2. \end{aligned} \tag{B6}$$

The term $\varepsilon_0|d_v|^2$ enters (B6) if $\tau_j \equiv k$, d_α's and d_v are given by (B3) and $\boldsymbol{\zeta}_D = \sum_{\alpha=1}^{3} d_\alpha \boldsymbol{\zeta}_\alpha$. We have also taken into account that due to (A6) $\sum_{\alpha=1}^{3}\frac{\partial d_\alpha}{\partial \tau_j}(\boldsymbol{\zeta}_D^\dagger \hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha) = 0$.

Due to (A6) $\boldsymbol{\zeta}_D^\dagger \hat{\mathbf{T}}\boldsymbol{\zeta}_D = 0$ for arbitrary purely real variables. In consequence the product $\boldsymbol{\zeta}_D^\dagger \hat{\mathbf{T}}\frac{\partial \boldsymbol{\zeta}_D}{\partial \tau_j}$ is purely imaginary, so Q_j is a purely real quantity.

APPENDIX C

The derivatives of $\det \hat{\mathbf{Z}}_{q\varepsilon}$ and b_{q_1} (22) at $\boldsymbol{\tau}_0$ can be cast into the form

$$\frac{\partial \det \hat{\mathbf{Z}}_{q\varepsilon}}{\partial \tau_j} = \frac{iQ_j}{b_3 \det \hat{\mathbf{U}}}, \quad \frac{\partial b_{q_1}}{\partial \tau_j} = \frac{1}{2g_{q_1'}^*}\left(\frac{\partial \boldsymbol{\zeta}_G^\dagger}{\partial \tau_j}\hat{\mathbf{T}}\boldsymbol{\zeta}_B\right), \tag{C1}$$

where

$$Q_j = i\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\left(\boldsymbol{\zeta}_\alpha^\dagger \hat{\mathbf{T}}\frac{\partial \boldsymbol{\zeta}_\beta}{\partial \tau_j}\right)b_\alpha^* b_\beta = i\left(\boldsymbol{\zeta}_B^\dagger \hat{\mathbf{T}}\frac{\partial \boldsymbol{\zeta}_B}{\partial \tau}\right), \tag{C2}$$

$$\boldsymbol{\zeta}_B = \sum_{\alpha=1}^{3} b_\alpha \boldsymbol{\zeta}_\alpha, \quad \boldsymbol{\zeta}_G = \sum_{\alpha=1,2,q_1,q_1'} g_\alpha \boldsymbol{\zeta}_\alpha, \tag{C3}$$

b_α's are given by (24) $g_\alpha = \det \hat{\mathbf{G}}_\alpha^*$, $\hat{\mathbf{G}}_\alpha = \mathbf{S}_{712v\beta}$, $\alpha = 1, 2$, and $\hat{\mathbf{G}}_\alpha = \mathbf{S}_{712v\alpha}$, $\alpha = q_1, q_1'$, and $\beta = \alpha + 4$ for $\alpha = 1, 2$. In (C2) we have taken into account the fact that due to (A6) $\sum_{\alpha=1}^{3}\frac{\partial b_\alpha}{\partial \tau}(\boldsymbol{\zeta}_B^\dagger \hat{\mathbf{T}}\boldsymbol{\zeta}_\alpha) = 0$. Note that the addend -$\varepsilon_0|d_v|^2$ arises in Q_j entering $\partial \det \hat{\mathbf{Z}}_{q\varepsilon}/\partial k$ and the addend $\det \hat{\mathbf{G}}_v/4k$, where $\hat{\mathbf{G}}_v = \mathbf{S}_{q_1 12vq_1'}$, enters $\partial b_{q_1}/\partial k$.

In the case of BIC-SAW2 the calculation of the derivatives of $\det \hat{\mathbf{Z}}_{q\varepsilon}$ and b_{q_m} (26) results in the expressions

$$\frac{\partial \det \hat{\mathbf{Z}}_{q\varepsilon}}{\partial \tau_j} = \frac{iQ_j}{b_2 \det \hat{\mathbf{U}}}, \quad \frac{\partial b_{q_m}}{\partial \tau_j} = \frac{1}{2g_{q_m}}\left(\frac{\partial \boldsymbol{\mu}_{q_m}^\dagger}{\partial \tau_j}\hat{\mathbf{T}}\boldsymbol{\zeta}_B\right), \tag{C4}$$

where

$$\begin{aligned} Q_j &= i\left(\boldsymbol{\zeta}_B^\dagger \hat{\mathbf{T}}\frac{\partial \boldsymbol{\zeta}_B}{\partial \tau_j}\right), \quad \boldsymbol{\zeta}_B = \sum_{\alpha=1}^{2} b_\alpha \boldsymbol{\zeta}_\alpha, \\ b_\alpha &= \det \hat{\mathbf{B}}_\alpha^*, \quad \alpha = 1, 2, \end{aligned} \tag{C5}$$

the matrix $\hat{\mathbf{B}}_\alpha$ is obtained from $\hat{\mathbf{B}}_{qm}$ (26) by replacing the last column $\mathbf{S}_\gamma$ by $\mathbf{S}_{\alpha+4}$, $\boldsymbol{\mu}_{q_1} = \sum_\alpha a_\alpha \boldsymbol{\zeta}_\alpha$, $\boldsymbol{\mu}_{q_2} = \sum_\beta c_\beta \boldsymbol{\zeta}_\beta$, the summation in $\boldsymbol{\mu}_{q_1}$ and $\boldsymbol{\mu}_{q_2}$ is carried out over $\alpha = 1, q_1, q_2, q_1'$ and $\alpha = 1, q_1, q_2, q_2'$, a_α and c_α are determinants of 5×5 matrices formed of S-vectors similarly to the above introduced 5×5 matrices, $g_{q1} \equiv a_{q'1}^*$ and $g_{q2} \equiv c_{q'1}^*$. One more term appears in $\partial \det \hat{\mathbf{Z}}_{q\varepsilon}/\partial k$ and $\partial b_{q_m}/\partial k$ because of the dependence of $\mathbf{S}_v$ (8) on k.

APPENDIX D

The effect of the crystallographic symmetry on the properties of the eigenvalues and eigenvectors of the transfer matrix in nonpiezoelectric periodic structures was analyzed in [49]. The same problem for piezoelectric structures may be approached similarly.

Owing to crystallographic symmetry the material constants and hence the matrix $\hat{\mathbf{N}}$ are invariant under certain transformations. For the cases listed in (27), the transformation matrices not changing the material constants may be written, respectively, in the form

$$\begin{aligned} &(1)\ \hat{\boldsymbol{\Delta}}_1 = \hat{\mathbf{I}} - 2\mathbf{n}\otimes\mathbf{n}, \quad (2)\ \hat{\boldsymbol{\Delta}}_2 = \hat{\mathbf{I}} - 2(\mathbf{m}\otimes\mathbf{m} + \mathbf{t}\otimes\mathbf{t}), \\ &(3)\ \hat{\boldsymbol{\Delta}}_3 = \hat{\mathbf{I}} - 2\mathbf{m}\otimes\mathbf{m}, \quad (4)\ \hat{\boldsymbol{\Delta}}_4 = \hat{\mathbf{I}} - 2(\mathbf{n}\otimes\mathbf{n} + \mathbf{t}\otimes\mathbf{t}), \end{aligned} \tag{D1}$$

where $\mathbf{t} = \mathbf{n}\times\mathbf{m}$. [Without piezoeffect options 1 and 2 in (27) are equivalent and so are options 3 and 4].

Using the fact that $\hat{\boldsymbol{\Delta}}_j^2 = \hat{\mathbf{I}}$, $j = 1, 2, 3, 4$, we find that the 4×4 matrices (nm), (nn) and (mm) (A2) satisfy the relations

$$\begin{aligned} (nm) &= -\hat{\boldsymbol{\Delta}}(nm)\hat{\boldsymbol{\Delta}}, \quad (nn) = \hat{\boldsymbol{\Delta}}(nn)\hat{\boldsymbol{\Delta}}, \\ (mm) &= \hat{\boldsymbol{\Delta}}(mm)\hat{\boldsymbol{\Delta}}, \end{aligned} \tag{D2}$$

where

$$\hat{\boldsymbol{\Delta}} = \begin{pmatrix} \hat{\boldsymbol{\Delta}}_j & \mathbf{0} \\ \mathbf{0}^t & 1 \end{pmatrix}, \quad j = 1, 2, 3, 4, \tag{D3}$$

and $\mathbf{0}$ is the 3×1 column of zeros. Hence due to (A2)

$$\hat{\mathbf{N}} = -\hat{\mathbf{K}}\hat{\mathbf{N}}\hat{\mathbf{K}}, \quad \hat{\mathbf{K}} = \begin{pmatrix} \hat{\boldsymbol{\Delta}} & \hat{\mathbf{0}} \\ \hat{\mathbf{0}} & -\hat{\boldsymbol{\Delta}} \end{pmatrix}. \tag{D4}$$

Let all the layers of the phononic crystal be oriented identically in accordance with one of the options listed in (27). In this instance the matrix $\hat{\mathbf{K}}$ is the same for all the layers, so, by virtue of (D4) and (A5) and the fact that $\hat{\mathbf{K}} = \hat{\mathbf{K}}^{-1}$, the transfer matrix $\hat{\mathbf{M}}$ (6) satisfies the relations

$$\hat{\mathbf{M}}^* = \hat{\mathbf{K}}\hat{\mathbf{M}}\hat{\mathbf{K}}, \quad \hat{\mathbf{M}}^{-1} = \hat{\mathbf{T}}\hat{\mathbf{K}}\hat{\mathbf{M}}^t\hat{\mathbf{K}}\hat{\mathbf{T}}. \tag{D5}$$

From (D5) it follows that if γ_α is an eigenvalue of the matrix $\hat{\mathbf{M}}$ then γ_α^{-1} is also an eigenvalue and if γ_α is an eigenvalue then γ_α^* is the eigenvalue corresponding to the eigenvector $\hat{\mathbf{K}}\boldsymbol{\zeta}_\alpha^*$, where $\boldsymbol{\zeta}_\alpha$ is the eigenvector corresponding to γ_α.

As a result, the eigenvalues associated with a pair of B modes $\alpha = i_n$ and $\alpha = r_n$ are complex conjugate, $\gamma_{r_n} = \gamma_{i_n}^*$. By virtue of the fact that $\hat{\mathbf{K}}\hat{\mathbf{T}}\hat{\mathbf{K}} = -1$, we may put

$$\boldsymbol{\zeta}_{r_n} = \hat{\mathbf{K}}\boldsymbol{\zeta}_{i_n}^* \tag{D6}$$

With this, the normalization relation (A9) holds true.

The eigenvalues associated with D modes may be purely real or complex. If γ_α is purely real then the eigenvalue $\gamma_{\alpha+4} = 1/\gamma_\alpha^*$ is also purely real and we have to put

$$\boldsymbol{\zeta}_\alpha = \hat{\mathbf{K}}\boldsymbol{\zeta}_\alpha^*, \quad \boldsymbol{\zeta}_{\alpha+4} = -\hat{\mathbf{K}}\boldsymbol{\zeta}_{\alpha+4}^* \tag{D7}$$

so as not to violate (A7). If γ_α is complex then there exist one more complex eigenvalue $\gamma_\beta = \gamma_\alpha^*$ and we put

$$\boldsymbol{\zeta}_\beta = \hat{\mathbf{K}}\boldsymbol{\zeta}_\alpha^*, \quad \boldsymbol{\zeta}_{\beta+4} = -\hat{\mathbf{K}}\boldsymbol{\zeta}_{\alpha+4}^*. \tag{D8}$$

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